HEFAT 2008
6th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics
30 June to 2 July 2008
Pretoria, South Africa
Paper Number: DC1

UNSTEADY ANALYSIS OF HYDROGEN/AIR MILD COMBUSTION BY MEANS OF LARGE EDDY SIMULATION

D. Cecere* , E. Giacomazzi , F. R. Picchia and N. Arcidiacono

*Author for correspondence
ENEA, Italian Agency for New Technologies,
Energy and Environment
Rome, Italy
E-mail: donato.cecere@casaccia.enea.it

ABSTRACT

Combustion processes are essential for power generation, since an overwhelming majority of energy-producing devices rely on the combustion of fossil or renewable fuels. Thus the development of a combustion technology able to accomplish improvement of efficiency with reduction of pollutant emissions, such as NO_x, is a main concern. MILD combustion is one of the promising techniques proposed to achieve these goals. In this combustion regime the reactants are preheated above the self-ignition temperature and enough inert combustion products are entrained in the reaction region. As a result, the characteristic times of chemical kinetics and turbulent mixing are comparable and the combustion region is no longer identifiable in a flame front but extended over a wide region, so that MILD combustion is often denoted as flameless combustion. Importantly, pollutants emissions can easily reduce because of the small temperature difference between burnt and unburnt and of the lean conditions in the combustion chamber. In this work Large Eddy Simulation (LES) of a Hydrogen/Air burner operating in the MILD combustion regime is performed. Turbulent mixing controls most of the global flame properties, so computing large scale structures by means of LES is an important key to capture mixing properties. The filtered mass, momentum, energy and species equations are discretized with a 2nd order accurate central finite difference scheme over a cylindrical non-uniform grid. Unclosed terms due to subgrid-scales are modeled using a fractal model approach (FM). Radiant transfer of energy is taken into account. The predictions of temperature and pollutant formation are compared with available experimental results.

INTRODUCTION

Since the influence of combustion products on the global climate had become a catchword in the discussion about the production of energy, the development of new technologies for a better utilization of fuels in terms of both thermal process efficiency and environmental impact is a major goal of combustion researchers.

The Moderate or Intense Low-oxygen Dilution (MILD) technology, also called flameless combustion, offers great advantages in terms of large energy savings with very low pollutant emissions. From a historical point of wiew, the technology was first named Excess Enthalpy Combustion, while today it is called High Temperature Air combustion (HiTAC), Flameless Oxidation (FLOX) and MILD [1]. It was stated that MILD combustion takes place when the temperature of the reactant mixture is higher than the mixture self-ignition temperature ($T_{inlet} > T_{si}$) and when the maximum temperature difference with respect to the inlet temperature is lower than the mixture self-ignition temperature in K [2]. The main operation principle for the MILD technique is the concept of hot exhaust gas recirculation, and consequently preheating and dilution of reactants. In fact, while the heat from the exhaust gases causes an increase of the temperature of the reactants, the exhaust gases dilute the mixture, reducing the oxygen concentration and maintaining low temperature in the combustion region [3; 4]. Furthermore, a massive recycle of the burnt gases is needed.

Due to its characteristics, a MILD process can easily control and level thermal gradients, thus avoiding the formation of hot spots in the combustion chamber and consequently, increasing the thermal capacity of the system, lowering thermal-NO_x and Soot production without compromising combustion efficiency. Because of small temperature gradients between burnt and unburnt gases, no extinction and ignition regions may be identified in MILD combustion regime. High-velocity jets of fuel, or of combustion air or of both fuel and oxidizer, create a low-pressure region close to the nozzle that promotes the mixing of the unburnt with a large amount of exhaust gases. As a result the combustion region is enlarged thanks to a fast dilution of the reactants and the final temperature is well below the adiabatic flame temperature. Since in MILD combustion processes temperature distribution is more homogeneous than classical combustion, materials used for the system are submitted to lower stresses.

The low chemical reaction rates due to high dilution in the combustion chamber makes chemical time scales comparable with that of turbulence (in fact MILD regime is located in the volumetric combustion region of the standard combustion diagram), challenging the applicability of combustion models that

assume fast chemistry like flamelet models (e.g., steady flamelet approach) and neglect differential diffusion effects. Coelho and Peters [5] simulated a furnace operating in the MILD regime applying flamelet approach in order to describe combustion/turbulence interactions. The models is unable to correctly describe residence time and the formation of NO_x, since this is a chemically slow process. Better results were achieved by means of unsteady flamelet modeling [4]. Christo and Dally, investigating numerically a jet in a hot coflow burner operating in MILD regime, showed that mixture fraction/flamelet models perform poorly for the MILD combustion and that molecular diffusion plays an important role both in the evaluation of temperature profiles and species concentrations [6]. In the present work the formulation adopted for the coupling of chemistry and turbulence in the LES simulation of the MILD combustion chamber, is based on the Eddy Dissipation Concept [7] and assumes that chemical reactions occur in small turbulent structures at the dissipation level and that the time evolution of concentration of chemical species in these structures is computed at each time step.

NOMENCLATURE

Y_i	$[-]$	Mass fraction of species i
μ	$[kg/ms]$	Dynamic viscosity
D_i	$[kg/ms]$	Dynamic diffusivity of specie i
Sc_i	$[-]$	Schmidt Number of species i
Δ	$[m]$	Local Filter Size
η	$[m]$	Kolmogorov Dissipative scale

THE BURNER AND NUMERICAL SET-UP

The burner is shown in Fig 1. It consists of a closed quartz cylinder divided in two sections: the combustion chamber (A) and the air preheating section (D). The core of the burner is a single high-velocity nozzle (B) with an internal diameter of 3 mm, inside which the fuel (Hydrogen in present case) stream is injected through a capillary pipe (C) perpendicularly to the primary air flow coming from (E). The chamber has a 25 mm internal radius and is 320 mm high. The chamber wall is electrically heated and its temperature set to a constant value of 1073 K. This is lower than that of the furnace to reduce the heat losses from the combustion chamber. At top the chamber is closed with a quartz plate that has three eccentric holes at 14 mm from the axis with a diameter of 10 mm and a central one of 4 mm, as shown in Fig 2. In the present case the inlet flow rate of secondary air (F) is set to zero. The lower section of the burner preheats the primary air thus simulating a recuperative heat exchanger.

Combustion air and fuel fully premix before entering the combustion chamber as demonstrated by previous RANS simulations of the complete high velocity nozzle and capillary pipe [9]. Once the primary air is mixed with the fuel and inert provided by the capillary pipe (C), the final inlet temperature is 517 K and the inlet velocity is 38.5 m/s resulting in a Reynolds number of 3261 (based on the jet diameter). The resulting high-velocity jet entrains a large amount of burnt gases from the combustion chamber and this provides the required fast dilution of reactants.

In order to evaluate the conditions at which MILD process takes place, the dilution factor inside the furnace, K_v, has an important key-role. This is defined as [8]

$$K_v = \frac{F_e}{F_a + F_f}, \tag{1}$$

that is related to the flow rate of fuel F_f, of the exhaust gases internally recirculated, and to the air flow rate F_a [11]. Following Derudi *etal*. [10], the corresponding value of K_v, calculated considering a value of the recycle factor $R = 5$, is 25.3. Following the definition of Cavigiolo [11], the recycle factor R imposed by the jet in the chamber is calculated as the ratio of the maximum value of the backflow rate to the inlet jet flow rate, by means of LES data and resulting in a value of 4.7. The numerical setup of the present simulation is reported in Table 1.

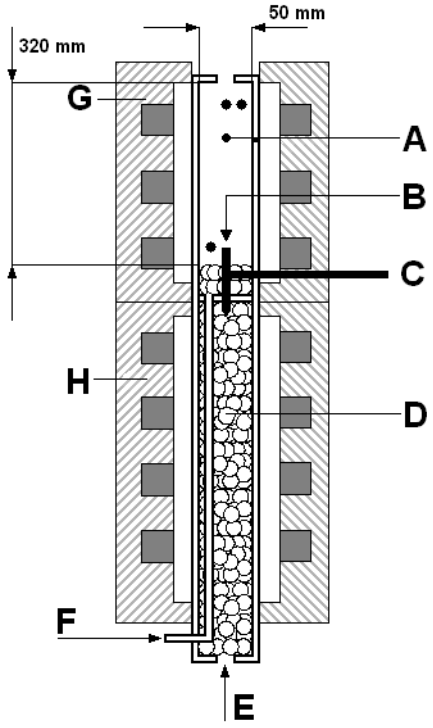

Figure 1. MILD burner layout: A, reaction chamber; B, nozzle; C, fuel inlet; D, preheating zone; E, primary air and inert gas inlet; F, secondary air inlet; G, upper oven for heat maintenance; H, preheating oven; (•) indicate thermocouple positions for temperature measurements.

NUMERICAL SIMULATION SET-UP

The experimental combustion chamber has three symmetry planes; therefore, LES simulation is performed on a sector of 120°. The computational grid is structured and has $636 \times 50 \times 45$ (1431000) nodes, respectively in the axial, radial and azimuthal direction.

Numerical simulations are performed by means of the in-house code HeaRT (Heat Release and Turbulence) using parallel computers available in ENEA computational grid [12]. For the present work explicit finite differences (convective and viscous CFL are 0.1 and 0.3 respectively), second order accurate in space (centered) and third order (Runge-Kutta) in time are

Table 1. Characteristics of the H_2/Air LES simulation.

H_2/Air MILD Simulation	
Inlet Velocity	38.9 m/s
Inlet Y_{H_2}	0.0038
Inlet Y_{O_2}	0.0309
Inlet Y_{N_2}	0.9653
T_{inlet}	517 K
T_{wall}	1076 K

used, to solve the fully compressible Navier-Stokes equations in cylindrical coordinate system. Explicit (non-linear) filtering of field variables is adopted to reduce numerical oscillations due to the centered spatial scheme [13], thus avoiding the requirement for a staggered grid. At the inlet, all quantities are prescribed, except pressure, that is obtained by a nil gradient condition. At the outlet, pressure is relaxed to a target value of 1 atm. This is achieved by implementing partially non-reflecting boundary conditions (NSCBC technique) to reduce numerical reflections of acoustic waves into the computational domain [26; 27]. All walls are assumed adiabatic, except the lateral wall of the combustor that is assumed at constant temperature, as in the experiments.

The perfect gas law is assumed as state equation. The detailed kinetic mechanism of Warnatz [14], involving 8 species and 37 reactions, is adopted in the present simulation.

MOLECULAR PROPERTIES

Molecular transports not taken into account in the resolved equations are: Dufour and Soret effects, cross-diffusion, pressure gradient diffusion, and diffusion by means of body force. Preferential diffusion is considered and the species diffusive mass flux is modeled by means of the Hirschfelder and Curtiss law [15].

All molecular properties for individual chemical species, except their binary mass diffusivities, are calculated a priori by using the software library provided by Prof. Ern (EGlib) [16; 17]. In particular, kinetic theory is used for dynamic viscosity [18, p. 23-29] and thermal conductivity [18, p. 274-278]. The calculated values are stored in a look-up table from 200 to 5000 K every 100 K. Values for intermediate temperatures are calculated at run-time by linear interpolation. The mixture-average properties are estimated at run-time. In particular, the simulations used in this work implement Wilke's formula with Bird's correction for viscosity [19] [20, p. 14], and Mathur's expression for thermal conductivity [21] [20, p. 15] The effective diffusion coefficients, D_i, of species i into the rest of mixture are estimated by means of assumed individual Schmidt numbers, Sc_i, calculated as the median of the Sc_i *vs* T distributions for nonpremixed flames [22].

SUBGRID MODELING

The unsteady simulations performed are based on the Fractal Model FM [23; 24; 25]. FM is an "eddy viscosity" subgrid model, turning itself off in the laminar regions of the flow. Turbulent energy cascade, from the local filter size Δ down to the local dissipative scale η, is modeled in each computational cell by means of a fractal (recursive) technique. FM assumes that chemical reactions take place only at the dissipative scales of turbulence (modeled as local Perfectly Stirred Reactors) and predicts the growth of these scales with increasing temperature. The filtered chemical source term is modeled by estimating the volume fraction γ^* occupied by the reactive "fine structures" and multiplying it by the local subgrid reaction rates. For the details of the FM model the reader is reminded to previous reference works [23; 24; 25].

The subgrid eddy viscosity involves a constant, σ_{FM}, assumed 0.1 in this work; subgrid turbulent thermal conductivity is estimated as $K_t = (\mu_t/\mu)K$; subgrid turbulent diffusivity by means of $D_{i,t} = (\mu_t/\mu)D_i$. These subgrid quantities are added to molecular ones.

RADIATION MODELING

Although radiative energy transport can strongly affect the thermo-fluid-dynamics of combustion, especially in large-scale turbulent flames, fires, and whenever soot is present, it is often neglected. MILD combustion is another situation where radiation is expected to play an important role in reducing peaks of temperature and spreading heat over wide portions of flow. In the present case, MILD combustion is realized burning hydrogen and this results in just one absorbing hot product, i.e., water, whose Planck absorption coefficient is lower than that of CO_2. Hence, despite the importance of radiation in MILD combustion in general, radiative heat transfer is expected to produce minor effects on hydrogen MILD combustion flow-field. In fact, in present work temperature increased by 20 K at maximum when radiation transfer was turned on.

A detailed description of radiation using, for instance, a discrete ordinate method is usually computationally very expensive. This is true for common RANS simulations, and it is much more true for LES simulations. In fact, up today in literature there is just one application of the ordinate method in LES [28]. To reduce computational cost radiation is commonly described using simplified models, such as the Milne-Eddington diffusion equation, valid in the limit of isotropic radiation, the Rosseland model, valid for high opacity media, or the optically thin model, valid for non absorbing media. Furthermore, turbulence-radiation interaction is typically neglected, although this has been found to be important, especially in pool fires [29].

In this work, a macroscopic radiation model, the M_1-model, also called the maximum entropy closure radiation model, is adopted. Since 1978 this model has been developed by many authors [30; 31; 32; 33; 34; 35; 36]. This model is founded on field equations for the radiative energy and the radiative heat flux vector. The limit is that it is valid for non scattering media. The main advantage is that it is independent of the opacity of the media, i.e., it adapts itself and works from thin to thick optical thickness. An averaged form of the M_1-model for turbulent flows also exists [37; 38], even though very complex and expensive to solve. A simplified formulation of this model was finally developed [39]: this is better suited for combustion problems and thus applied in present simulations. Partial differential equations involved in the model are hard to be solved numerically. To this aim, it is assumed that radiation equilibrates very quickly, i.e., quasi-steady Radiative Transfer Equations are solved (by using a SOR technique coupled to a median spatial filter) periodically at some time steps to update the radiative sink/source term in the transported energy equation.

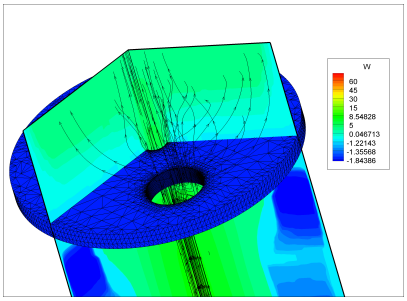

Figure 2. Particular of the exit section of the combustion chamber and velocity streamtraces.

IMMERSED BOUNDARY METHOD

Since the computational grid used in the present simulation is structured it would not be possible to manage complex geometries. In particular, the top of the combustion chamber is closed by means of a disk with three eccentric holes and a central one. This disk, shown in Fig. 2 was modeled by using the Immersed Boundary Method (IBM). This method has recently been successfully applied to complex geometries without requiring additional computational cost and without sacrificing accuracy [40; 41].

With this technique the treatment of momentum and scalar equations in complex geometric configurations is possible on structured meshes by means of forcing conditions on surfaces corresponding to the physical location of the complex boundaries. The forcing condition depends on the location and the fluid velocity and thus it is a function of time. Its location, x_i is not generally coincident with the grid and the forcing must be extrapolated to these nodes. The forcing is zero inside the fluid and is non-zero in the cells near the immersed boundary. Consider the $N-S$ equations discretized in time, e.g.,

$$\frac{\widetilde{u_i}^{n+1}-\widetilde{u_i}^{n}}{\Delta t} = \mathrm{RHS_i}^{n+1/2} + f_i^{n+1/2}, \qquad (2)$$

where $\mathrm{RHS_i}^{n+1/2}$ contains convective, viscous terms and the pressure gradient. The boundary conditions can be either Dirichlet or Neumann types. Extrapolating the velocity (V^{n+1}) and pressure fields in the cell near the immersed boundary using nearby fluid points and associated boundary information the value of the forcing $f_i^{n+1/2}$ to be imposed is:

$$f_i^{n+1/2} = -\mathrm{RHS_i}^{n+1/2} + \frac{\mathrm{V}^{n+1}-\mathrm{u_i}^{n}}{\Delta \mathrm{t}}. \qquad (3)$$

This forcing causes the desired boundary condition to be satisfied at every time step. The boundary conditions implemented near the solid boundaries are no slip conditions for velocities and zero gradient for pressure, temperature and other scalars.

RESULTS AND DISCUSSION

The flow topology is characterized by a wide recirculation region that has its own dynamics. This contributes to preheating and mixing of inlet reactants. Temperature and radical H distributions are shown in Fig. 3 and 4. Figure 5 shows the radial profiles of temperature at different heights in the combustion chamber. As shown temperature varies only in the preheating region of the core jet and shows a constant profile in

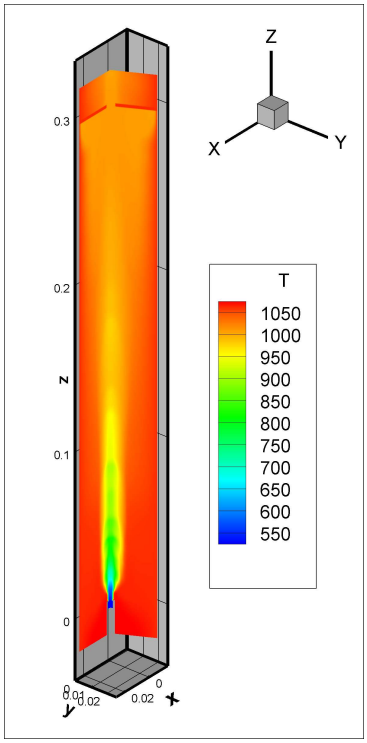

Figure 3. Instantaneous temperature profile in the MILD combustion chamber (K).

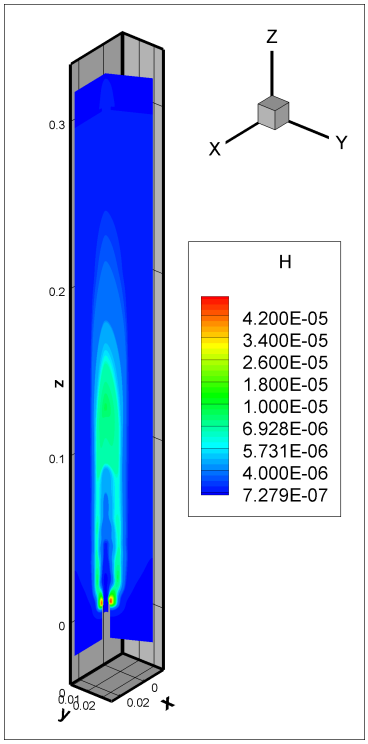

Figure 4. Instantaneous mass fraction profile of the species H in the MILD combustion chamber.

zones where recirculation phenomena hold. In the experiments, temperature was measured by means of thermocouples at three locations, as indicated in Fig. 1. The positions and the comparison with numerical prediction are shown in Table 2. The experimental temperature measurements are affected by an error of 50K related to the system of measurement and to the error on the position of the probe in the combustion chamber [43].

The maximum temperature value in the combustion chamber is around 1050K and a maximum difference of 110K be-

tween measured and numerical results is shown in Table 2. In agreement with these low temperatures, a posteriori calculation showed very low NO_x concentrations ($\sim 1ppm$) at the exit section of the combustion chamber. Temperature history was sampled at different locations in the combustion chamber: these data revealed that the flow experiences a maximum fluctuation of the order of 2% with respect to the mean value in zones where combustion-turbulence interaction is stronger. These maximum fluctuations are less than those reached in standard flames.

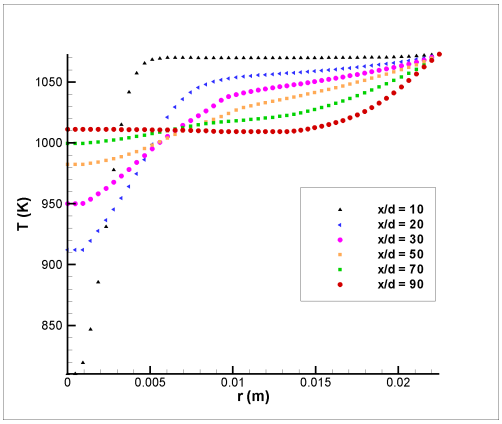

Figure 5. Radial profiles of temperature at different heights above the nozzle ($d = 3mm$).

Table 2. Comparison between experimental and numerical temperature predictions.

Z $[m]$	r $[m]$	Degree	T_{exp}(K)	T_{num}(K)
0.275	0.	60	1121	1012
0.145	0.014	60	1132	1036
0.080	0.010	60	1168	1046

The classical definition of MILD is based on external parameters such as the characteristics of the inlet mixture and the maximum temperature in the combustion system. The high momentum of the inlet mixture in the combustion chamber ensures high scalar dissipation rates closer to the jet exit (order of 200 s^{-1}), that promotes mixing of the fuel with exhaust gases. We can assume that locally near the nozzle the inlet mixture is fed towards the hot gases that transfer their enthalpy to the fresh mixture. In order to understand what are the possible effects of turbulence on the flame structures in the MILD regime a series of simulations on a laminar counterflow diffusion flame at different values of the strain rate is performed by means of the module OPPDIFF of CHEMKIN software [42], with the kinetic mechanism of Warnatz [14] and results shown in Fig. 6. A premixed hydrogen-air flow, with the same composition and temperature of the inlet mixture used for the present combustor, is fed towards an opposed flow of nitrogen at higher temperature (1100 K) that simulates the hot recirculating gas in the combustor. Figure 6 reports temperature distribution versus mixture fraction. It is observed that temperature slowly varies in function of the strain rate K. It is stressed that this weak dependence of temperature on strain rate is due to the high dilution of actual inlet mixture.

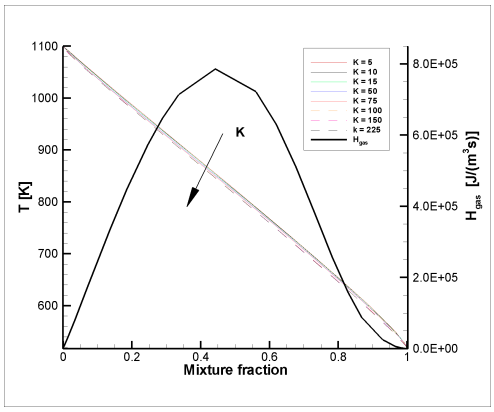

Figure 6. Temperature profile versus mixture fraction at different values of strain rate $\mathrm{K} = \mathrm{V}/\mathrm{D}$ in a laminar diffusion counterflow flame. V is the velocity in the counterflow configuration and D is the distance of the two entraining jets. H is the heat release rate ($J/m^3 - s$).

The same figure also reports the heat release rate. Its distribution evidences that the regime is based on the autoignition of the mixture due to enthalpy diffusion from the inert flow. In fact, this regime is characterized by oxidation in a broad mixture fraction range. Finally, this demonstrates that capturing the local mixing due to molecular diffusion in MILD regime is crucial. Since LES is more effective than RANS in estimating local molecular diffusive processes (being not hidden by unphysical turbulent viscosity), this makes Large Eddy Simulation as the best candidate to simulate MILD combustion. Furthermore, this conclusion is more true for less diluted inlet mixture that are more influenced by local strain rate effects.

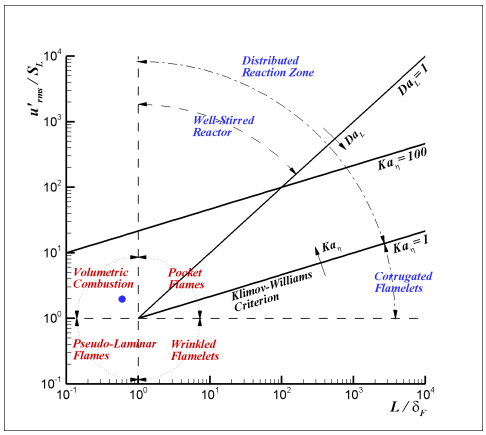

Figure 7. Borghi's diagram.

The MILD regime of the present burner can be represented by a single point on the standard combustion diagram. The quantities required to define this point are the laminar flame speed, S_L, the flame thickness, δ_F, the integral macroscale, L and its associated rms velocity, u'_{rms}. To derive these quantities attention was focused on a sampling point close to the nozzle, representative of MILD conditions. The laminar flame speed ($\sim 10\,\mathrm{cm/s}$) was derived from the laminar counterflow diffusion flame previously analyzed, by taking the flow velocity at

the location of maximum heat release. As flame thickness was assumed the length of the preheating region of the inlet mixture, equal to 5 mm; it is observed that this length can be deduced both from LES flowfields (e.g., see Fig. 5, $x/d = 10$) and from temperature profiles of laminar counterflow diffusion flame calculations. The integral macroscale ($L \sim 3\,mm$, that is of the same order of magnitude of the injector diameter) was estimated by multiplying the time-frequency (~ 66 Hz) corresponding to the low frequency peak in the kinetic energy spectrum and the associated velocity fluctuation (~ 0.2 m/s). Thus, the point representative of present MILD regime is characterized by $u'_{rms}/S_L = 2$ and $L/\delta_F = 0.66$, as shown in Fig. 7.

CONCLUSIONS

A numerical investigation by means of Large Eddy Simulation of a burner operating in the MILD combustion mode has been presented. MILD combustion unsteady simulation has evidenced high scalar dissipation rate near the nozzle that promotes mixing with hot inert gases and dilution of the inlet mixture. Laminar flame calculations evidenced that the local scalar dissipation rate, for the present inlet mixture, affects weakly temperature distribution but strongly enthalpy diffusion from the inert flow. Only in the region close to the inlet, steep temperature gradients appear while a rather homogeneous temperature field, characterized by very low fluctuations, is observed in the whole combustion chamber.

ACKNOWLEDGMENT

Thanks to Roberto Verzicco, Professor at University "TorVergata" in Rome, for his helpful discussions on the implementation of the Immersed Boundary method. Thanks also to Antonio Cavaliere, Professor at University "Federico II" in Naples for his helpful discussions on MILD combustion.

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